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by Fe⁺ Ions

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Pulsed ion-beam synthesis of β -FeSi₂ layers on Si implanted by Fe⁺ ions

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Abstract. Synthesis of β -FeSi₂ layers on Si was performed by high-dose Fe⁺ implantation in Si at 300 K with subsequent pulsed ion treatment (PIT) on implanted layers by powerful ion beams (PIB) of nanosecond duration. It was shown that the layer consists of the grains (presipitates) β -FeSi₂ with size approximately 30–40 nm. The results of the optical absorption indicate the formation of direct-band gap structures with an optical gap $E_g \sim 0.82$ – 0.83 eV. It is shown that the pulsed ion-beam synthesized sample is able to emit at the $\lambda \sim 1.56$ μ m up to temperature of 210 K.

Introduction

Recently the formation of Si-based structures emitting in the visible and near infrared (IR) spectral region attracts essential interest. There are two main approaches to the fabrication of structures emitting in the wavelength $\lambda \sim 1.55$ μ m: formation of Si:Er and β -FeSi₂ layers. β -disilicide is a direct-band material with an optical gap $E_g = 0.8$ – 0.9 eV [1]. This gap value corresponds to the optical wavelength $\lambda \sim 1.45$ μ m which is close to the technologically important $\lambda \sim 1.55$ μ m corresponding to the absorption minimum of the silica optical fibers. This fact allows one to create optoelectronic devices in the near IR region integrated in the silicon microelectronic technology.

One of the main approaches for the formation of buried layers of low-defect, emitting β -FeSi₂ is an ion-beam synthesis (IBS) i.e. high-dose Fe⁺ implantation in Si with subsequent high-temperature and long-duration annealing ($T = 800$ – 900°C , $t \sim 20$ h) [2, 3].

In this work an influence of pulsed ion treatment (PIT) by powerful ion beams (PIB) on the implanted Si layers in order to synthesize β -FeSi₂ is investigated.

1. Experimental

Single-crystalline n-type Si wafers with (100) orientation were implanted by Fe⁺ ions at room temperature (RT) with energy of 40 keV and dose of $1.8 \cdot 10^{17}$ cm⁻² (ion current density of 5 $\mu\text{A}/\text{cm}^2$). One part of implanted samples was subjected to PIT on a TEMP accelerator (C⁺, H⁺, $E = 300$ keV, $\tau = 50$ ns, $j \sim 50$ A/cm²) and the other part was thermally annealed (TA) in N₂ ambient (800°C, 2.5 h) to compare the results.

Crystallographic structure of implanted and annealed layers was studied by glancing x-ray diffraction technique (XRD) on a diffractometer with an iron anode ($\lambda = 1.93$ Å). IR spectroscopy in the reflection and transmission mode was employed to determine the band gap energy. In photoluminescence (PL) measurements optical excitation was provided by an Ar⁺ laser ($\lambda = 514.5$ nm) with an average excitation power of 50 mW. PL signal was registered with a liquid nitrogen-cooled Ge photodiode (North Coast).

2. Results and discussion

X-ray characterization. After ion implantation no reflections are present in XRD pattern (not shown) indicating that complete amorphization of the implanted layer takes place. Figure 1 shows XRD patterns of the samples subjected to various treatment regimes after ion implantation. From Fig. 1(a) one can see that after PIT mixing of two phases takes place: the metallic FeSi and semiconducting β -FeSi₂. The most intensive peak in the spectrum belongs to the β -FeSi₂ phase with indistinguishable reflections (220)/(202) due to proximity of their positions.

In order to remove the lattice strain and to transform the residual amount of FeSi phase into β -FeSi₂ a short-time TA (800°C, 20 min) in N₂ atmosphere was performed. XRD pattern after additional TA is shown in Fig. 1(b). From this figure one can see the essential increase of (220)/(202) β -FeSi₂ peak intensity. In the inset of Fig. 1(b) is shown an azimuth dependence of (220) peak indicating the presence of the [110] texture in the silicide layer. To compare results Fig. 1(c) shows the XRD pattern of the implanted sample after long-time TA (800°C, 2.5 h). In this case the formation of β -FeSi₂ with unstrained lattice and [110] texture (inset of Fig. 1(c)) The XRD patterns were evaluated by using the MAUD program. It was obtained that these layers consist of the grains (presipitates) with the size 30–40 nm.

Optical characterization. Since the dependence of the absorption coefficient (α) on the photon energy (E) for the direct interband transitions it is given by [4]: $\alpha = A(E - E_g)^{1/2}$, where A is a constant that is associated with specific features of the band structure and E_g is the magnitude of the direct band gap, then drawing up the dependence of the absorption exponent $(\alpha d)^2$ on E (d is the silicide thickness) according to the equation $\alpha d = \ln(1 - R)/T$, one can determine the E_g value extrapolating the straight line up to the intersection with the E axis (Fig. 2). E_g values (~ 0.82 eV for the sample only after

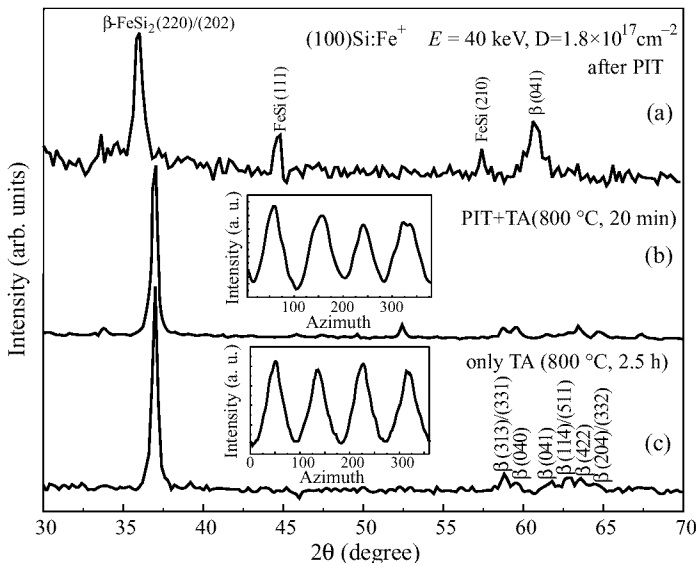


Fig. 1. XRD patterns of the implanted sample ($E = 40$ keV, $D = 1.8 \times 10^{17}$ Fe⁺/cm⁻²) after PIT (C⁺, H⁺, $E = 300$ keV, $\tau = 50$ ns, $j \sim 50$ A/cm²) (a), after PIT with additional TA (800°C, 20 min) (b), only after TA (800°C, 2.5 h) (c). In the insets are shown an azimuth dependencies of β -FeSi₂ (220)/(202) peak intensity.

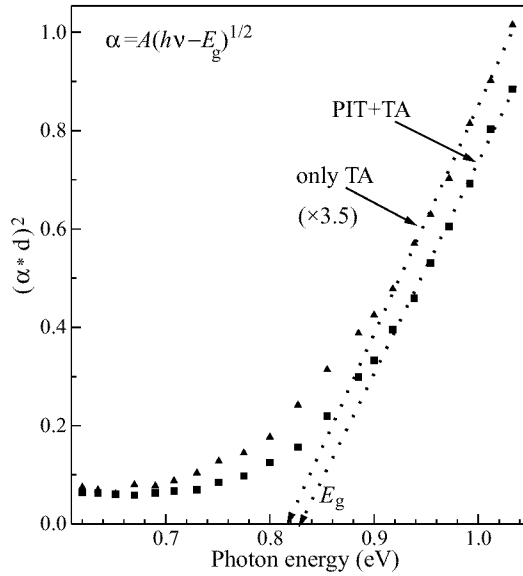


Fig. 2. Square of absorption exponent vs photon energy for the implanted sample after PIT with short-time TA and only after long-time TA.

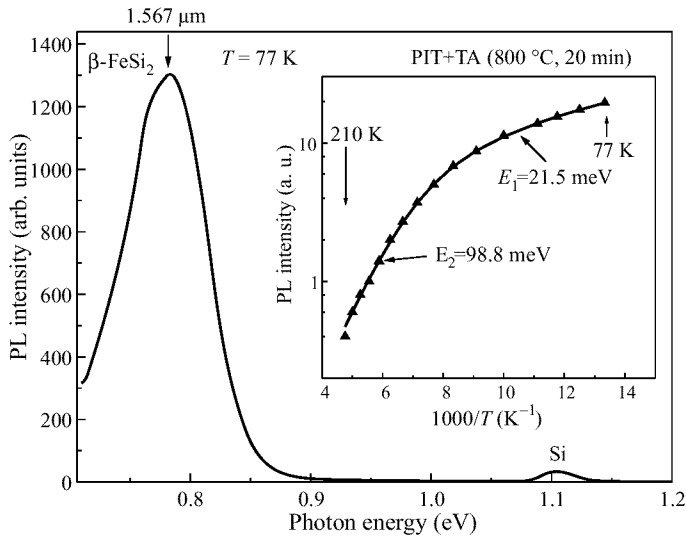


Fig. 3. PL spectra of the implanted sample after PIT with short-time TA. Inset shows a temperature dependence of PL intensity (solid circles) and the theoretical data fitting by Eq. (1).

TA and ~ 0.83 eV after PIT and TA) correspond to the E_g values of β -FeSi₂ given in the literature [3].

Figure 3 shows the PL spectrum measured at 77 K in the implanted sample after PIT and additional TA (800°C, 20 min). One can see two emission bands corresponding to the PL signal from the Si substrate ($E \sim 1.10$ eV) and from β -FeSi₂ ($E \sim 0.785$ eV - $\lambda \sim 1.567$ μ m). The PL signal is observed up to $T = 210$ K by about 40–50 K exceeding

the maximum temperature which is reached by other authors on the samples prepared by the traditional IBS method [3]. In the inset of Fig. 3 the temperature dependence of the PL intensity of the sample after PIT and TA is shown. The equation describing a PL quenching curve has a two-exponential form [5]:

$$I(T) = \frac{I_0}{1 + C_1 \exp[-(E_1/kT)] + C_2 \exp[-(E_2/kT)]}, \quad (1)$$

where I_0 is the saturated PL intensity at very low temperature, C_1 and C_2 are the coupling coefficients, E_1 and E_2 are the thermal annealing energies. E_1 and E_2 are values at which Eq. (1) most satisfactorily describes the experimental data and they were determined to be 21.5 and 98.8 meV, respectively.

The origin of the PL signal is one of the problems associated with the light emission in the region of $\lambda \sim 1.55 \mu\text{m}$. It is known that when a dislocation network and $\beta\text{-FeSi}_2$ phase are simultaneously present in a sample it is necessary to disentangle the contribution of $\beta\text{-FeSi}_2$ and dislocations to the $1.55 \mu\text{m}$ luminescence [6]. Thermal quenching energy values for the registered PL signal differ from those for the D1 dislocation center ($\sim 7\text{--}12 \text{ meV}$) [7] whose energetic position ($E \sim 0.81 \text{ eV}$) is very close to the PL maximum position ($E \sim 0.785 \text{ eV}$). Because of this we conclude that the origin of the PL signal at the $\lambda \sim 1.56 \mu\text{m}$ is not connected with the dislocation-related emission and is caused due to the direct interband transitions in a $\beta\text{-FeSi}_2$ optical gap.

3. Conclusions

We have shown that the PIT of Fe^+ -implanted layer leads to the mixing of two phases (FeSi and $\beta\text{-FeSi}_2$) with a strained state of the crystal lattice. Subsequent short-time TA (800°C , 20 min) results in the complete transformation of FeSi phase into $\beta\text{-FeSi}_2$ with the production of a highly textured layer. It was shown that these layers consist of the grains with size 30–40 nm. The results of the optical absorption indicate the formation of direct-band gap structures with an optical gap $E_g \sim 0.82\text{--}0.83 \text{ eV}$ in both cases. It is shown that the pulsed ion-beam synthesized sample is able to emit at the $\lambda \sim 1.56 \mu\text{m}$ up to temperature of 210 K. From the results of PL signal temperature dependence the light emission at the $\lambda \sim 1.56 \mu\text{m}$ was attributed to the direct interband transitions in the $\beta\text{-FeSi}_2$ optical gap with thermal quenching energies of 21.5 and 98.8 meV.

The result demonstrates the potential of $\beta\text{-FeSi}_2$ as an important candidate for a silicon-based optoelectronic technology.

Acknowledgments. This work was supported by NIOKR Foundation of Tatarstan Republic, Russian Federation (grant No 16-03). The authors would like to thank V. A. Shustov for his experimental support in X-ray measurements.

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